MMSNF-2003

TECHNICAL PROGRAM

Materials Modeling and Simulations for Nuclear Fuels

June 9-10, 2003

Santa Fe, New Mexico, U. S. A.

Los Alamos NATIONAL LABORATORY

MONDAY, June 9

Santa Fe Room

8:15 Welcome and Announcements

Programmatic Context (Chair K. Chidester)

8:30 E. Arthur (NTA Office) The Six Laboratory Director Nuclear Initiative -- How Advanced Fuels Development Supports its Objective.

9:00 K. Pasamehmetoglu (AFCI Office) Overview of AFCI Fuel Development.

9:30 Discussion

9:45 COFFEE BREAK

Session A: Modeling and Simulation Scales (Chair R. Grimes)

10:15 J. Wills (LANL) Prediction of Materials Properties for Nuclear Fuels from First Principles Calculations.

10:40 M. Baskes (LANL) The Role of Atomistic Modeling in Designing Materials.

11:05 M. Stan (LANL) Continuum Scale Simulations in Support of Nuclear Fuels Development.

11:30 Discussion

12:00 LUNCH, ***Coronado*** Room

Santa Fe Room

Session B: Thermodynamic Properties (Chair J. Wallenius)

1:30 A. Niklasson (LANL) Modeling the Actinides with Disordered Local Moments.

1:55 S. M. Valone (LANL) Charge Fluctuation Models for Nuclear Fuels Properties.

2:20 S.G. Srivilliputhur (LANL) Atomistic Modeling to Develop New Nuclear Fuels: A Case Study Using the Am-N System.

2:45 Discussion

3:00 COFFEE BREAK

Session C: Phase Stability (Chair J. Simmons)

3:30 P. Mason (AEA Technology, US/UK) Solidus and Liquidus Determinations for a UO_{2+x}-ZrO_2 Mixture.

3:55 M. Jolkkonen (KTH, Sweden) Decarburisation Reactions Modelled using Thermo-Calc and the ALCHYMY Database for Uranium-Free Fuels.

4:20 T. C. Wallace (LANL) Phase Stability in Materials for Nuclear Fuels Applications.

4:45 Discussion

5:00 Announcements

6:00 BANQUET, ***Coronado*** Room

MMSNF-2003
TECHNICAL PROGRAM

TUESDAY, June 10

Santa Fe Room
8:15 First Day Summary and Announcements
Session D: Thermo-Mechanical Properties (Chair W. Ching)
8:30 I. Han (Arizona State Univ.) Micro-Hardness, Fracture Toughness, Fatigue and Texture Development in Sintered ZrN.
8:55 A. Zubelewicz (LANL) Micromechanics Based Characterization of Deformation Mechanisms and Damage in Heterogeneous Fuel-like Materials.
9:20 J. H. Simmons (Univ of Arizona) MD Simulations of Fracture in Silica - Effects at High Temperature.
9:45 J. Tulenko (Univ. of Florida) FRAPCON: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup.
10:10 Discussion
10: 30 COFEE BREAK

Session E: Transport Phenomena (Chair M. Baskes)
11:00 S. P. Chen (LANL) First Principles Calculations of the Transport Properties in Materials.
11:25 P. Cristea (LANL) Defect Thermochemistry of Nonstoichiometric Metal Oxides.
11:50 Discussion

12:00 LUNCH, ***Coronado*** Room

Santa Fe Room
Session F: Irradiation Effects (Chair J. Tulenko)
1:30 W. Ching (Univ. of Missouri-Kansas City) Spectroscopic Signatures of Defected Ceramics.
1:55 J. Wallenius (KTH, Sweden) Atomistic Modelling of Radiation Damage in Fe-Cr alloys.
2:20 R. Grimes (Imperial College, UK) Fission Product Accommodation and Containment.
2:45 Discussion
3:00 COFFEE BREAK

Session G: The Impact of Modeling and Simulations on Nuclear Fuels Development (Chair E. Arthur)
3:30 K. Chidester (LANL) Coupling Experiments and Simulations for Designing Materials for Nuclear Fuels.
3:45 Discussion: Modeling and Simulations in Support of Nuclear Fuel Development and Qualification.
4:45 Summary of the workshop.
5:00 Final Announcements and Goodbye.

For information regarding the Technical Program please contact Marius Stan (mastan@lanl.gov) or visit the workshop web page at: http://www.lanl.gov/mst/nuclearfuels/